# A Kondo impurity in one dimensional correlated conduction electrons

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A spin-$\frac{1}{2}$ magnetic impurity coupled to a one-dimensional correlated electron system have been studied by applying the density renormalization group method. The Kondo temperature is substantially enhanced by strong repulsive interactions in the chain, but changes non-monotonically in the case of electron attraction. The magnetization of the impurity at zero-temperature shows local Fermi liquid behavior.

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During the last decade, much effort has been devoted to the investigation of the electron-correlation effects. They are present most prominently in the copper-oxide materials which display high-$T_c$ superconducting and unusual normal-state properties [1] and may even show heavy-fermion behavior [2]. In one dimension (1D), an interacting electron system is known to be a Luttinger liquid [3]. It seems possible that in the future by means of quantum wire fabricated by nanotechnique one can study the effect of magnetic impurities on Luttinger liquid [4] .

The problem of a Kondo impurity coupled to a Luttinger liquid was first considered by Lee and Toner [5]. By using perturbative renormalization group theory they found that the Kondo temperature $T_K$ depends on the coupling $J$ between the impurity and the conduction electrons in the form of a power law (not exponential) provided that the interaction between electrons is sufficiently strong compared to $J$. Because of the neglect of local backscattering their treatment does not preserve SU(2) symmetry. The local backscattering was included within the poor man's scaling by Furusaki and Nagaosa [6] who obtained a stable strong coupling fixed point for $J > 0$ as well as $J < 0$. Moreover, by employing a $1/J$ expansion, they found that a temperature expansion of thermodynamic quantities shows critical behavior, i.e., *non-integer exponents*. It is an open question though, how well such a perturbative expansion is justified in the strong coupling regime. In fact, a simplified model [7] for conduction electrons, which consists of right-moving spin-up and left-moving spin-down electrons, leads to the conclusion that the Kondo impurity behaves like a local Fermi liquid [8]. On the other hand, boundary conformal field theory methods [9,10] result in two types of critical behavior, i.e., either a local Fermi liquid or one of the form proposed in [6]. Most recently, Chen et al [11] predicted local Fermi liquid behavior by making use of the parity and spin-rotation symmetry of the problem.

The above literature indicates that the critical behavior of a Kondo impurity coupled to a Luttinger liquid is not fully understood yet. One scenario would be that of a local Fermi liquid but with a substantially enhanced $T_K$ due to strong correlations between conduction electrons. For example, the characteristic energy scale in the heavy fermion system $Nd_{2-x}Ce_xCuO_4$ is much larger than expected for Kondo ions coupled to free electrons [12].

In this paper, we study ground-state properties of a Kondo ion antiferromagnetically coupled to a 1D Hubbard model by applying the Density Matrix Renormalization Group (DMRG) [13]. The Hamiltonian is:

$$\hat{H}_0 = -t\sum_{i,\sigma}[\hat{c}^{\dagger}_{i\sigma}\hat{c}_{i-1,\sigma} + \mathrm{h.c}] + U\sum_{i}\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + J\hat{\mathbf{S}}\cdot\hat{\mathbf{s}}_0$$

where $\hat{\mathbf{S}}$ is the impurity spin, $\hat{\mathbf{s}}_0$ an electron spin at $i = 0$ and other notations are standard. In the limit of $U = \infty$ and half-filling, the problem reduces to one of an impurity coupled to a Heisenberg antiferromagnetic chain, a system studied before (see Refs. [14–16]). Here we will consider all $U$ values and band fillings equal to as well as different from one-half.

The Kondo problem is concerned with the question of how the magnetic moment of the impurity is suppressed by decreasing temperature $T$ or external magnetic field $H$. The critical behavior of a magnetic impurity shows up in the low-$T$ thermodynamics *and also* low-$H$ properties [17–20]. Here we would like to determine the latter for $T = 0$. For that purpose, we calculate the spin susceptibility $\chi_0$ of the impurity at $H = 0$ and the magnetization of the impurity for various values of $H$. The former gives rise to the energy scale (the Kondo temperature) $T_K$ or alternatively the screening length $\xi_K$ ($\chi_0 \propto 1/T_K \propto \xi_K$). The field-dependent magnetization $M(H)$ exhibits the critical behavior of the system, since it contains a term proportional to $(H/T_K)^\alpha$ with $2 < \alpha \leq 3$ for small $H$. This can be used to distinguish between a local Fermi liquid [7,11] or an anomalous response case [6]. As the field is applied exclusively to the impurity spin, we add $\hat{H}_M = -H\hat{S}_z$ to $\hat{H}_0$. By using the Hellmann-Feynman theorem, we have $M(H) = \langle\Psi_0(H)|\,\hat{S}_z\,|\Psi_0(H)\rangle$ where $|\Psi_0(H)\rangle$ is the ground state in the presence of $\hat{H}_M$, and $\chi_0 = [\partial M(H)/\partial H]_{H=0}$. $\chi_0$ is numerically evaluated as the coefficient of the linear term in an $H$-expansion of $M(H)$. For given $J$ and $U$, the values of $H$ is chosen so small, for instance $H = 0.00015$ at $J = 0.5$ and $U = 20$,

that the contributions from higher orders in $H$ are negligible in comparison with numerical errors (see below).

The application of the DMRG method to inhomogeneous systems as considered here is not straightforward because local couplings must be properly renormalized by DMRG procedures [21]. Let us discuss briefly some essential points involved in our studies. The number of states kept mostly is between 256 and 512. The truncation errors are the order of $10^{-10}$. In order to work with a non-degenerate ground state, our system consists of one impurity and an odd number of conduction electrons $N$. The filling factor $\nu = N/L$ ($L$: the number of sites) equals one, for which DMRG calculations are performed with odd $L$ under open boundary conditions, if not stated otherwise, but values of $\nu = 1/2$ and $3/4$ and correspondingly an even number of sites $L$ are also considered with periodic boundary conditions. When $L = 4k+1$ ($k$ being an integer) and the impurity is located to the centre of the chain the ground state has total spin $S^{tot} = 0$ [22]. In this case, the two sites which are added in each DMRG step have maximum distance to the impurity, and at least three *sweeps* are taken when the calculations are performed. In the presence of $\hat{H}_M$, the ground state is again taken in the $S_z^{tot} = 0$ subspace. Systematic relative-errors based on truncations are estimated to be the order of $10^{-7}$. DMRG calculations are done for chain lengths $33 \leq L \leq 105$ so that independent extrapolations show relative deviations between $10^{-4}$ and $10^{-3}$. We consider those as the systematic relative-errors of our final results.

The spin of a Kondo ion is compensated by a spin screening cloud surrounding the ion [23]. When $U = 0$, the 1D system is metallic. The screening length $\xi_K$ is then related to the Kondo temperature $T_K$ via $\xi_K \approx v_F/T_K$ where $v_F$ is the Fermi velocity. When $J\rho \ll W$ where $W$ is the band width and $\rho = 1/2\pi$ is the density of state at the Fermi level ($t = 1$ in our calculation), it is $\xi_K \approx a e^{1/J\rho}/\sqrt{J\rho}$. For $T_K \sim 10K$, the screening length extends over thousand lattice spacings $a$. The strong correlations between conduction electrons decrease $\xi_K$ *substantially*. Figs. 1(a), and (b) show $\chi_0 \sim \xi_K(J)$ [also $\chi_0^{-1} \sim T_K(J)$] for $U = 0$, and 20, respectively. i) *a crossover:* Consider first Fig. 1(a). In order to reach the thermodynamic limit, we must have $L \gg \xi_K/a$. This limits us to $J \geq 2$. The figure suggests a crossover from a strong coupling to a weak coupling at $J \approx 2.5$. In Fig. 1(b), the same crossover takes place at approximately $J \approx 0.4$. ii) *a weak coupling regime:* Note that for $J = 0.3$ we find $\chi_0 = 3.73$ for $U = 20$ while for $U = 0$ we obtain $\chi_0 \sim 10^5$ [23]. iii) *a strong coupling regime:* One also notices from Fig. 1(a), and (b) that for large values of $J$ it is $T_K \sim J$. The linear dependence sets in for $U = 20$ at much lower values of $J$ ($J \gtrsim 1$) than for $U = 0$ ($J \gtrsim 40$). These features on the energy scale $T_K$ support previous findings [5–7,9,11].

In Fig. 2, we shows $\chi_0$ as a function of $U$ for $J = 4$. For $U \gg W$, the exchange coupling between sites in the chain $J_{ex} = 1/4U$ becomes much smaller than $J$, implying that a singlet which extends over *a few lattice spacings* is formed between the spins of the magnetic ion and the chain. $\chi_0$ saturate at $1/2J$ as $U \gg W$, which corresponds to a local singlet between the spins of the ion and the lattice site 0. The situation differs in the case of electron attraction ($U < 0$). One notices a maximum in $\chi_0$ at $U_c \approx -1.0$. For $U_c(J) < U < 0$ the effective Kondo coupling is reduced by the attractive electron-electron interaction, and $\xi_K$ is enhanced. With increasing attraction electrons form more and more on-site pairs. When $|U|$ becomes much larger than the binding energy of the Kondo singlet and than $W$, all the electrons are paired except one (remember that $N$ is an odd number). This unpaired electron forms a singlet with the magnetic impurity so that $\chi_0$ saturate in the limit $U \to -\infty$ [24]. Moreover, close to $U = 0$, the susceptibility $\chi_0$ is *linear in* $U$, which confirms perturbation results for $T_K$ [25]. When both $J\rho$ and $|U|$ are much smaller than $W$, one can approximately transform the problem into one of an impurity coupled to free electron with an effective Kondo coupling given by $J^z_{eff} = J + U/4$ and $J^{\perp}_{eff} = J$. It is i) $J^z_{eff} > J^{\perp}_{eff} > 0$ when $U > 0$ [11]; ii) $0 < J^z_{eff} < J^{\perp}_{eff}$ when $U_c < U < 0$; iii) $J^z_{eff} < 0$ and $J^{\perp}_{eff} > 0$ when $U < U_c$. This classification explains qualitatively the behavior of $\chi_0$ in Fig. 2 in the relevant range of $U$. To explore the behavior of $\chi_0$ around $U_c$, we have calculated several values of $U$ near $U_c$. As shown in Fig. 2, the curvature close to $U_c$ reveals, with a relative error $\lesssim 10^{-4}$, that $U_c$ is a crossover rather than a critical point.

It is elucidating to study in more details the different states between the impurity and the site 0, which appear in the $|\Psi_0(H=0)\rangle$ as well as their weights. They are constructed from the impurity-spin states $\{|\uparrow\rangle, |\downarrow\rangle\}$ and the spin states $\{|0\rangle_0, |\uparrow\rangle_0\, |\downarrow\rangle_0, |\uparrow\downarrow\rangle_0\}$ of site 0, from which we can form a singlet $|\psi_s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_0 |\downarrow\rangle - |\downarrow\rangle_0 |\uparrow\rangle)$; a triplet $|\psi_t\rangle = \{|\uparrow\rangle_0 |\uparrow\rangle, \frac{1}{\sqrt{2}}(|\uparrow\rangle_0 |\downarrow\rangle + |\downarrow\rangle_0 |\uparrow\rangle), |\downarrow\rangle_0 |\downarrow\rangle\}$; and a quadruplet $|\psi_q\rangle = \{|\uparrow\downarrow\rangle_0 |\uparrow\rangle, |\uparrow\downarrow\rangle_0 |\downarrow\rangle, |0\rangle_0 |\uparrow\rangle, |0\rangle_0 |\downarrow\rangle\}$. We extract the these states from $|\Psi_0(H=0)\rangle$ by making use of a reduced density matrix. The corresponding probabilities are $P_s$, $P_t$ (for each of the three states) and $P_q$. When $U \ll U_c$, one finds $P_s \gg P_t$ and $P_q \gg P_t$, and also has $P_s \gg P_q$ if $J$ is a sufficiently large. The following results are found when $U \geq 0$: i) for $U \lesssim W$, one finds $P_s \geq P_q \geq P_t$; ii) for $U \gg W$, it is $P_s \geq P_t \geq P_q$. When in addition, $J_{ex} \gg J$, we obtain $P_s \sim P_t \gg P_q$, indicating that the impurity spin is almost fully polarized by the strong correlated electrons in the chain. In contrast, when $J_{ex} \ll J$, we find $P_s \gg P_t \gg P_q$, implying that a local Kondo singlet is formed. Two examples are given in Fig.3 for $U = 20$ and $J = 0.0005, 0.5$ where also correlation functions $\langle\Psi_0(H=0)|\, \hat{S}^z \hat{s}^z_i \,|\Psi_0(H=0)\rangle$ are shown as a function of $i$. The correlations are long ranged, particularly for small values of $J$.

The magnetization of the impurity is well suited for studying the critical behavior of the system under investigation. Shown in Fig. 4 is the impurity magnetization $M$ as functional $\chi_0 H$ ($\sim H/T_K$) for various values of $J$ and $U$. The solid line corresponds to the expected behavior in the strong coupling limit, i.e., $M(\chi_0 H) = \chi_0 H/\sqrt{1+4(\chi_0 H)^2}$. One notices that the data fall onto a universal curve with slight but systematic deviations for $\chi_0 H \gtrsim 10^{-1}$ (see inset). Two different regimes are clearly distinguishable, a strong coupling regime for lower values of $\chi_0 H$ and a weak coupling regime in which the magnetization is saturated at $M = 1/2$. [17–19] In the strong coupling regime the impurity spin is well compensated by the spins of the electrons in the chain, while in the weak coupling regime the singlet is broken by $H \geq \chi_0^{-1}$. The deviations are natural even for $U = 0$, since the calculations are performed in real space without any assumption on the density of states and the values of $J$ are not much smaller than $W$ [26]. This however does not change the universality class. Particularly, for small values of $\chi_0 H < 10^{-1}$, i.e., the critical behavior, $M(\chi_0 H)$ behaves in the same way for *positive and negative* $U$ and *small and large* $J$ values at $\nu = 1$. For the case of $\nu \neq 1$, let us consider the lower field behavior quantitatively. According to [6], one might expect that for small fields $H$, $M(\chi_0 H) = \chi_0 H + \alpha_1 (\chi_0 H)^{1/K_\rho + 1} +$ higher orders in $H$. When $U$ is finite and $\nu \neq 1$, one has $1/2 < K_\rho < 1$. It turns out that $\chi''(\chi_0 H) = \partial^3 M/\partial(\chi_0 H)^3$ should become *singular* at $H = 0$ if the above conjecture as regards $M(\chi_0 H)$ holds. In this case, a scaling analysis is valid. For finite $L$, the original question becomes whether $\chi_0''(\chi_0(L)H) \propto [\chi_0(L)H]^{\alpha(K_\rho(L))}$ *with or without* the size-dependent $K_\rho(L)$ for the Hubbard model, i.e., $\chi_0''(\chi_0(L)H)$ is divergent as $\chi_0(L)H \to 0$ *if and only if* $K_\rho(L)$ appear in $\alpha(K_\rho(L))$. We have computed $\chi''(0)$ for $\nu = 1/2$, $3/4$, and $1$ by the exact diagonalization for the length $L$ up to 12. $\chi''(\chi_0 H)$ is accurately evaluated order by order in a numerical way with the use of $\frac{\mathrm{d}f(x)}{\mathrm{d}x} \sim (f(x) - f(x - \delta x))/\delta x$ for sufficiently small $x = \chi_0(L)H$ and $\delta x = \chi_0(L)\delta H$. For instance, at $\nu = 3/4$ ($L = 12$), $U = 0.5$, and $J = 0.01$, $\chi''(x) = -12.000173$, $-12.000157$, $-11.999287$ $-11.996831$, and $-11.971354$ for $x = 1.476262 \times (10^{-5}, 10^{-4}, 10^{-3}, 2\times 10^{-3}, 6 \times 10^{-3})$, respectively, and $\delta x = 6.6020 \times 10^{-5}$. We found that $\chi''(\chi_0 H) = -12.00$ at $H = 0$ is *independent of* the values of $\nu$, $U$ ($U$ = 0, 0.5, 10) and $J$ ($J$ = 0.01, 0.5, 5). For a larger system of $L = 33$ and $N = 25$, we obtained $\chi''(\chi_0 H = 0) = -11.5$ by the DMRG calculation with keeping 800 states and nine sweeps. Note that although this result is less accurate than that given by the exact diagonlaization, it is *still finite*. The above analysis turns out that $\alpha(K_\rho(L))$ equals to zero exactly in the same way as for the case $U = 0$ [27]. Therefore, $M(\chi_0 H) = \chi_0 H - 2(\chi_0 H)^3 +$ higher orders in $H$ as described by a local Fermi liquid.

In conclusion, we have studied the ground state properties of a magnetic impurity coupled to an interacting 1D system of conduction electrons. We found that a local Fermi liquid picture is still valid but that the characteristic energy scale, i.e., $T_K$ is substantially enhanced by the strong repulsive interaction in the chain and affected non-monitonically in the case of electron attraction. We infer the validity of a local Fermi liquid description from the fact that the magnetization $M(\chi_0 H)$ shows the same critical behavior for $U = 0$ and for $U \neq 0$.

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[27] We note here that the size-dependent $K_\rho(L)$ does not appear in the exponent of $H$ in the small $H$ expansion *but* is non-trivially hidden in $\chi_0(L)$ which associates the screening cloud with $K_\rho(L)$.

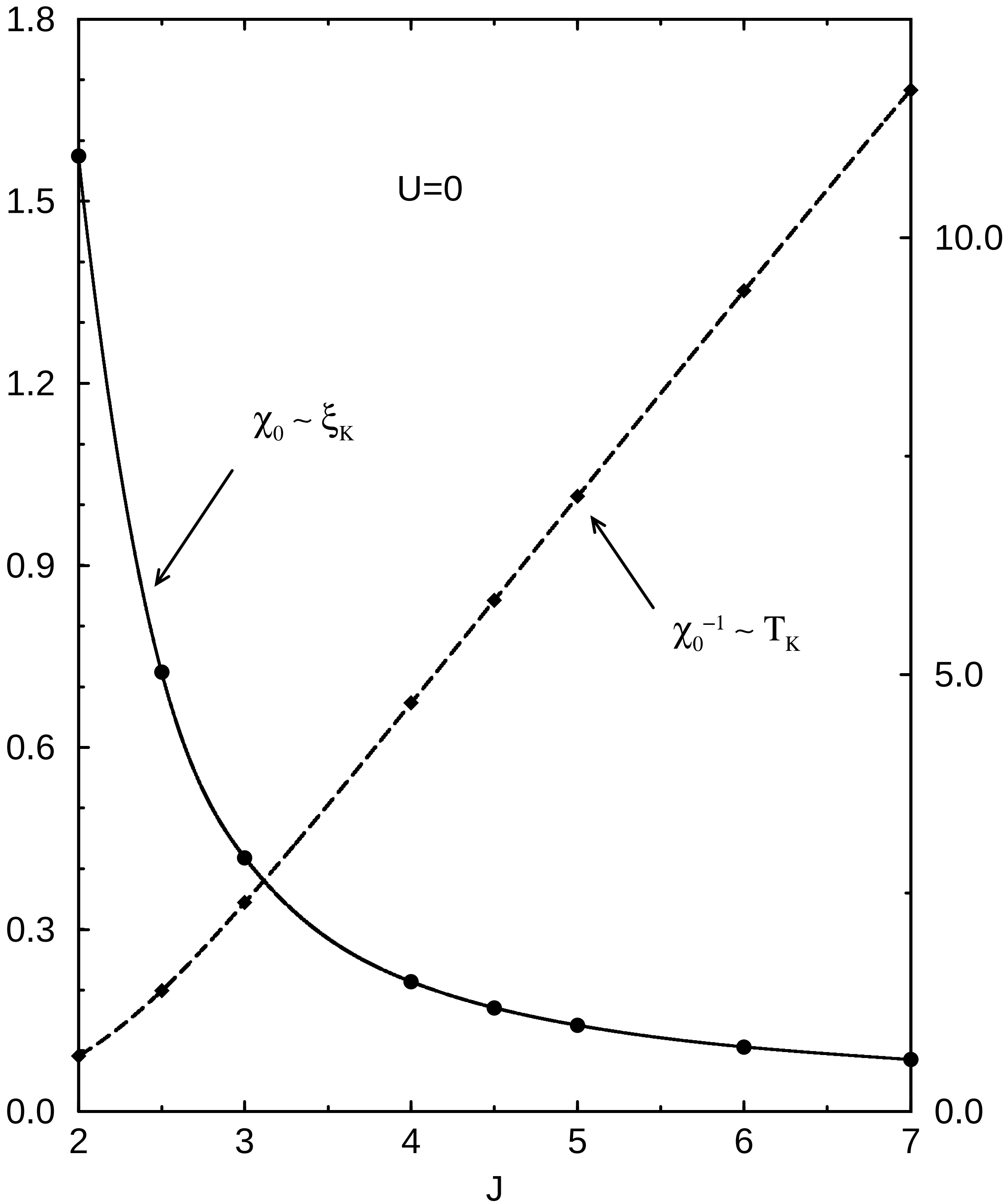
FIG. 1. (a) $\chi_0 \sim \xi_K$ and $\chi_0^{-1} \sim T_k$ *vs* $J$ at $U = 0$. The left vertical axis is for $\chi_0$ and the right one for $\chi_0^{-1}$. (b) The same as (a) but at $U = 20$. The fit-curves are guides to the eye (Solid curve and the filled circles are for $\chi_0$ and Dashed-line curve and the filled square for $\chi_0^{-1}$).

FIG. 2. $\chi_0$ *vs* $U$ at $J\rho = 2/\pi$. The fit-curves are guides to the eye.

FIG. 3. Correlation functions between the impurity spin and electron spins, and the local states between the impurity and the spin at $i = 0$ for $J = 0.0005, 0.5$ at $U = 20$.

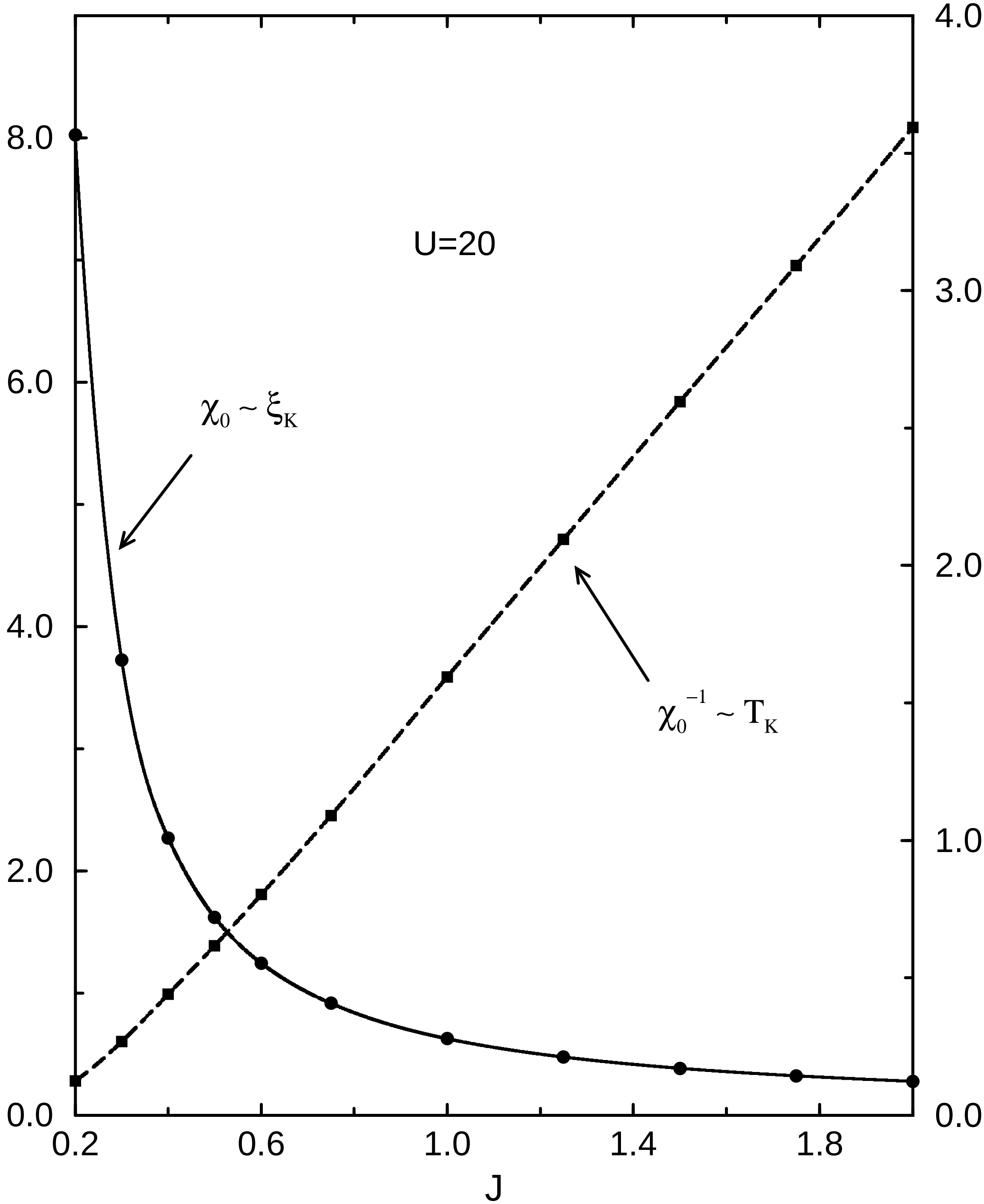
FIG. 4. $M(\chi_0 H)$ *vs* $\chi_0 H$. The solid curve is for strong coupling limit. Each kind of symbols for a given set of $J$ and $U$. Inset: the amplified crossover regime.

Fig. 1a



1.8
1.5
1.2
0.9
0.6
0.3
0.0
10.0
5.0
0.0
2
3
4
5
6
7
J
U=0
$\chi_0 \sim \xi_K$
$\chi_0^{-1} \sim T_K$

Fig. 1b



U=20
$\chi_0 \sim \xi_K$
$\chi_0^{-1} \sim T_K$
8.0
6.0
4.0
2.0
0.0
4.0
3.0
2.0
1.0
0.0
0.2
0.6
1.0
1.4
1.8
J

Fig. 2

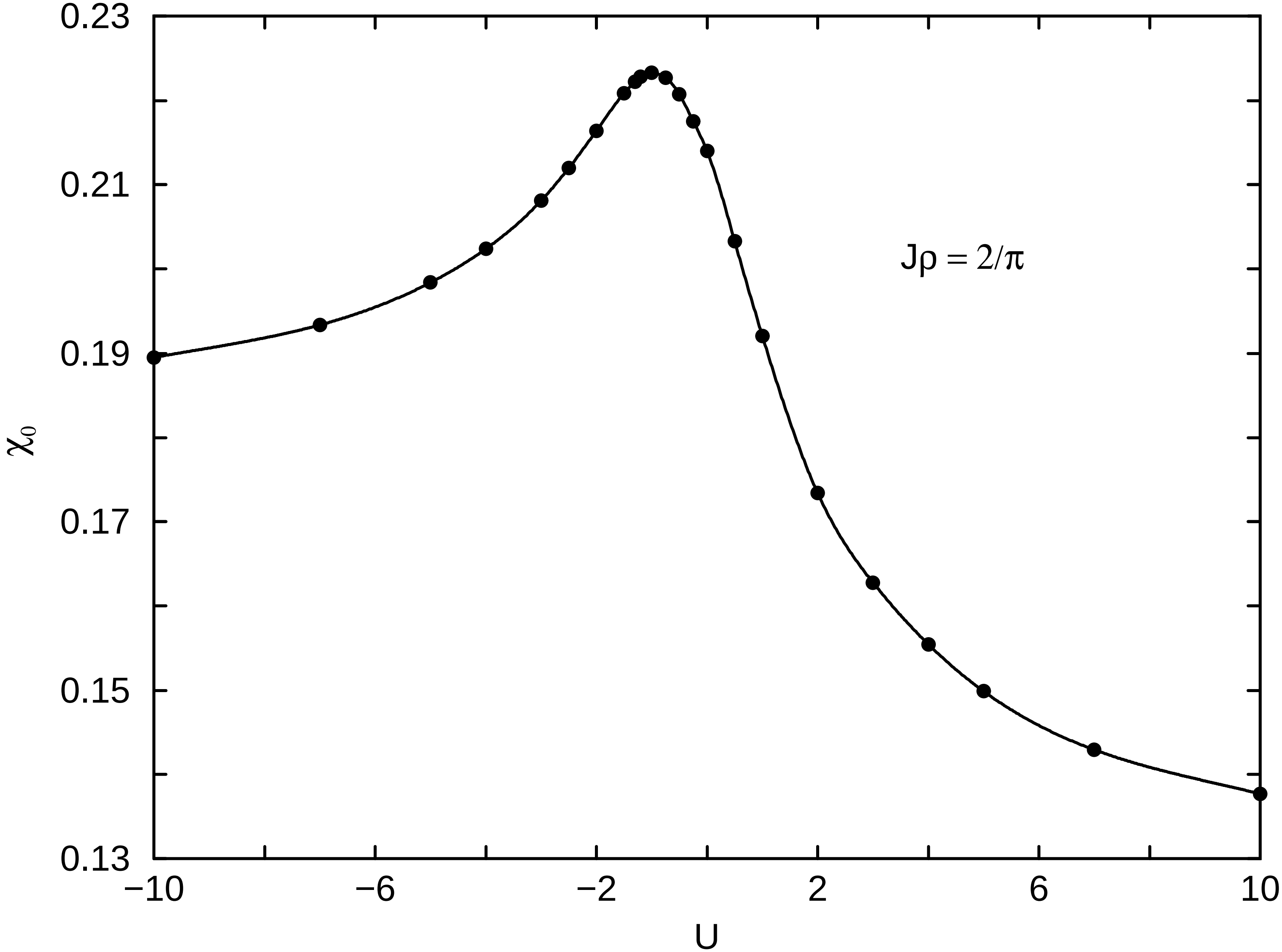
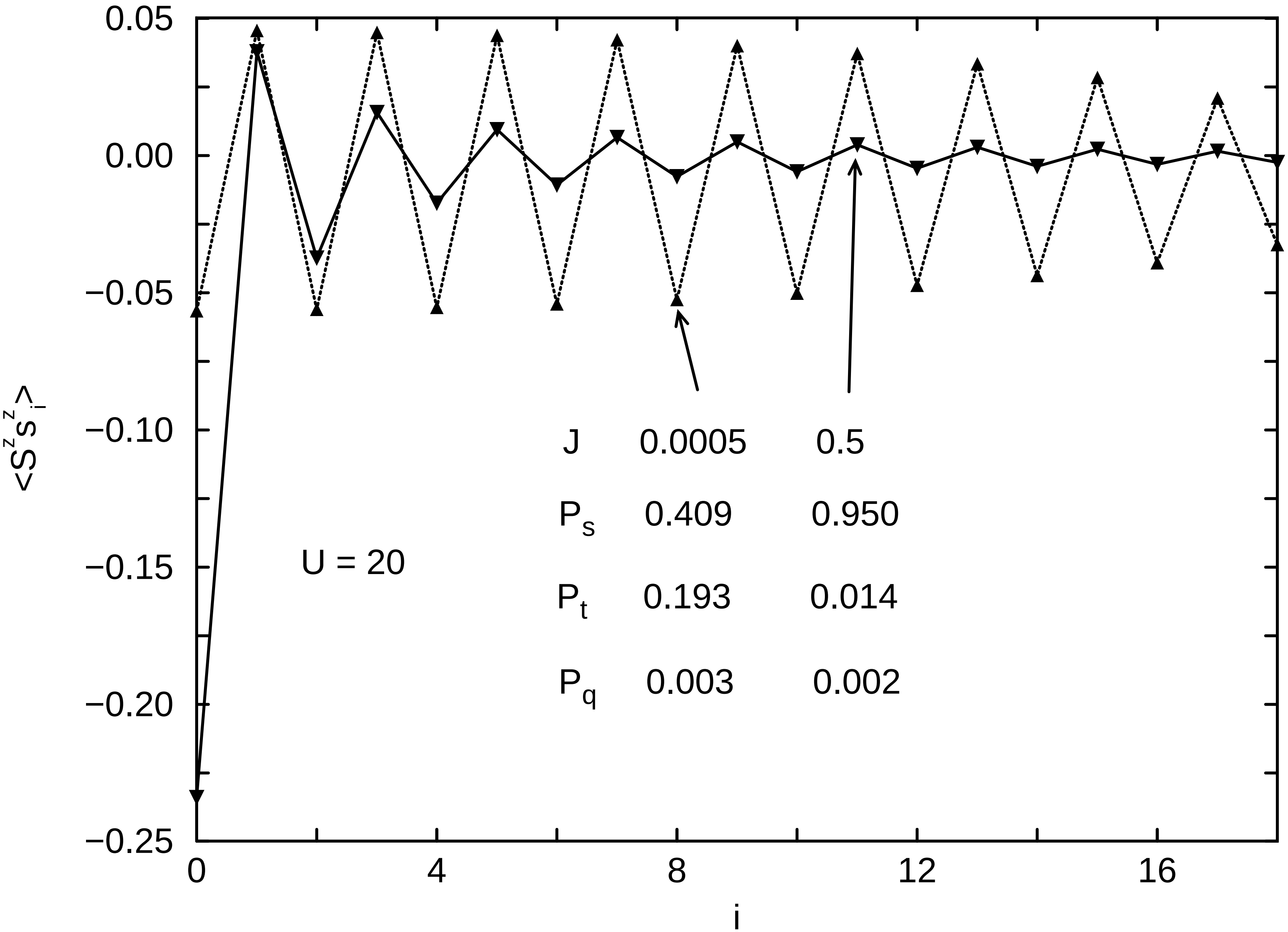
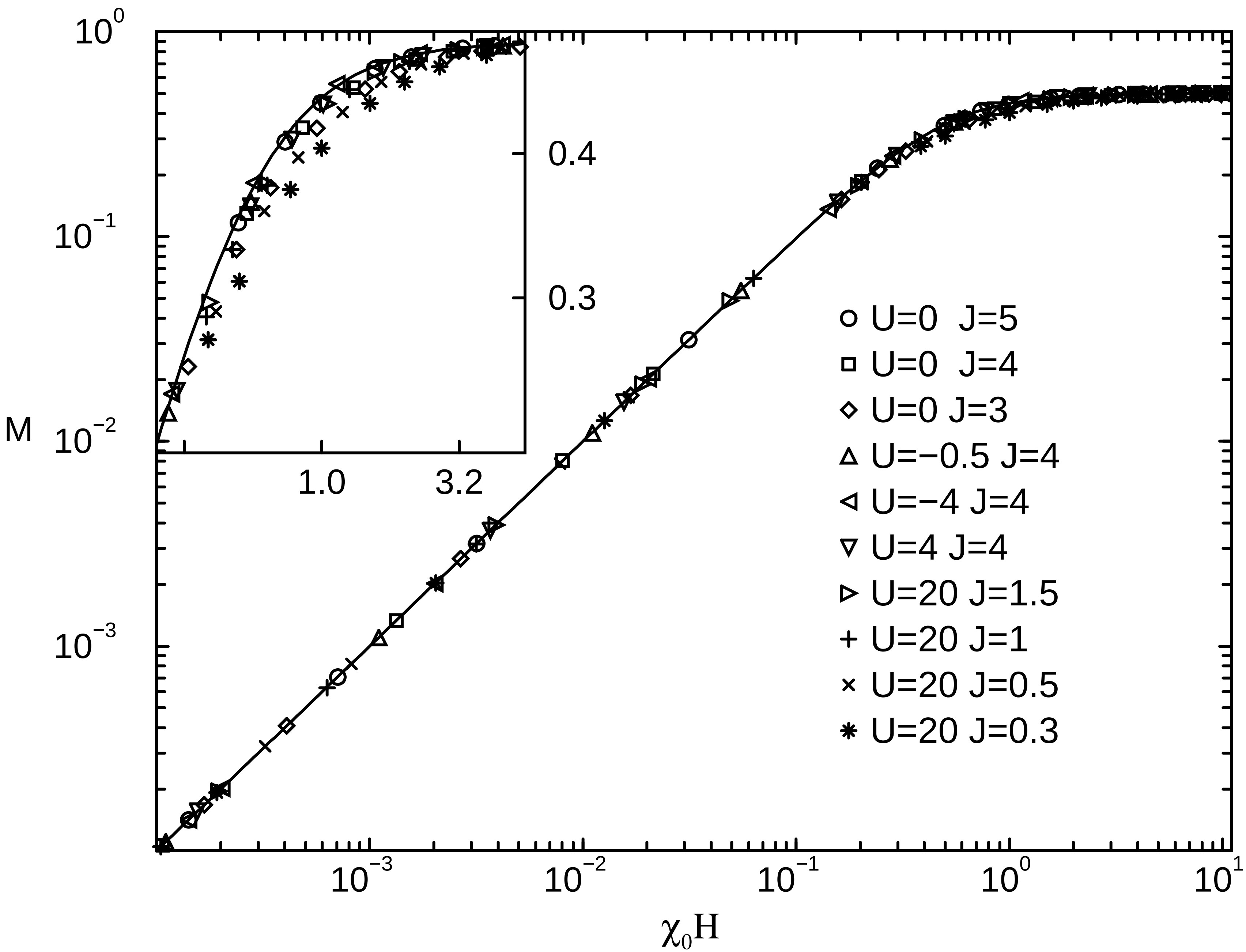


Fig. 3



0.05
0.00
−0.05
−0.10
−0.15
−0.20
−0.25
0
4
8
12
16
i
$\langle S^z s^z_i \rangle$
U = 20
J 0.0005 0.5
$P_s$ 0.409 0.950
$P_t$ 0.193 0.014
$P_q$ 0.003 0.002

Fig. 4



M
$\chi_0$H
U=0 J=5
U=0 J=4
U=0 J=3
U=−0.5 J=4
U=−4 J=4
U=4 J=4
U=20 J=1.5
U=20 J=1
U=20 J=0.5
U=20 J=0.3